LA-UR-07-3363 May 15, 2007

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Title: Micro-Gap Experiments and Insensitive Explosives

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Submitted to: | APS Topical Conference

**Shock Compression of Condensed Matter** 

Waikoloa, HI

June 24 – July 29, 2007



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## MICRO-GAP EXPERIMENTS AND INSENSITIVE EXPLOSIVES

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**Abstract.** Early research on shock desensitized plastic-bonded explosives (circa 1970) also studied large single crystals of explosive. High quality crystals — free from voids that serve as nucleation sites for hot spots — have been found to be very insensitive to shock initiation. In fact, experiments were not able to initiate a 10 mm crystal of HMX with a detonation wave in PBX 9404, which is 94 weight % HMX. Yet a single crystal of the same size can be initiated by a flyer plate that drives a shock wave at about the Chapman-Jouguet pressure of PBX 9404 or 35 GPa. This is especially puzzling since the detonation wave in PBX 9404 has a peak pressure at the von Neumann spike of nearly 60 GPa. An important difference between the two drive systems is a small gap at the PBX 9404/HMX interface due to surface roughness of the PBX; estimated to be about 30 microns. Conceptually, the experiment is equivalent to the gap test used to compare the sensitivity of explosives; albeit with a micro-gap and a very insensitive explosive. The inability of a PBX 9404 detonation wave to initiate a single crystal of HMX is due to the reaction zone in the PBX 9404 being of comparable length to the gap and the rarefaction or Taylor wave behind the detonation front.

**Keywords:** PBX 9404, HMX crystal, gap test, shock initiation

**PACS:** 47.40.-x,47.70.Fw

## INTRODUCTION

Experiments have shown that a weak shock can desensitize and even quench a propagating detonation wave in a plastic-bonded explosive (PBX); see for example Campbell & Travis[1]. This emphasized the critical role that hot spots play in the initiation of a heterogeneous explosive.

Pressing moulding powder (explosive grains coated with binder) into a PBX leads to a small amount of porosity; for example, 1 to 2 per cent of the volume in the HMX based PBX 9404. As a test of the hypothesis that void collapse is the dominant hot-spot mechanism for shock initiation of a PBX, experiments were performed in the 1970's on large void-free single crystals of HMX. These experiments showed that, compared to PBX 9404, a crystal of HMX is very insensitive to shock initiation.

One set of experiments by Campbell & Craig [see fig. 5 of ref. 1] found that a detonation wave in PBX 9404 did not initiate HMX. Subsequent exper-

iments by Craig [see table 4 of ref. 1] found that a 35.8 GPa shock driven by a flyer plate did initiate HMX but that a slightly weaker shock of 34 GPa did not initiate a 7.4 mm crystal. Since the Chapman-Jouguet pressure of PBX 9404 is 35 GPa and the von Neumann spike pressure is up to 60 GPa, it is puzzling that a detonation wave in PBX 9404 would not initiate HMX.

Measurements of the reaction zone of PBX 9501, which like PBX 9404 has a high HMX content, provide a key clue. The data show that the reaction zone is very narrow, about  $30 \,\mu \text{m}$ ; see [2] and references therein. Moreover, the reaction zone width is comparable to the expected surface roughness of PBX 9404. The surface roughness is due to the soft binder material and the bimodal size distribution of the HMX grains; machining a piece of PBX to size would likely knock out some fine grains which have an average size of about  $30 \,\mu \text{m}$ . An indication of surface roughness is the loss of reflected light in VISAR experiments unless a thin plastic buffer is placed be-

tween the PBX and the window.

Modeling the surface roughness with an inert gap leads to an experimental configuration (detonation wave in donor explosive, gap, acceptor explosive) analogous to that of the gap test used to determine the relative sensitivities of different explosives. As the gap is increased the effective initiation pressure for the acceptor decreases due to the Taylor wave behind the detonation front in the donor. The acceptor explosive is sensitive to shock initiation if the maximum gap size (for which the acceptor can be detonated) is large. In contrast, a small maximum gap size corresponds to an insensitive explosive.

For the Campbell & Craig experiments, the donor explosive is PBX 9404 and the acceptor explosive is HMX. The micron-scale gap is significant because it prevents the high von Neumann spike pressure of the donor detonation wave from being transmitted to the acceptor and the HMX induction time gives rise to an initiation threshold (for the crystal lengths used) near the CJ pressure of PBX 9404.

Simulations presented in the following sections show that the above perspective is a viable explanation for the failure of a detonation wave in PBX 9404 to initiate a crystal of HMX.

#### **SIMULATIONS**

The initiation experiments were designed to be essentially one-dimensional; the PBX is initiated with a plane wave lens and the length to width of the PBX and crystal are less than 1. The exception is the PBX surface roughness, for which the interface with HMX can be modeled as a gap or thin layer of inert.

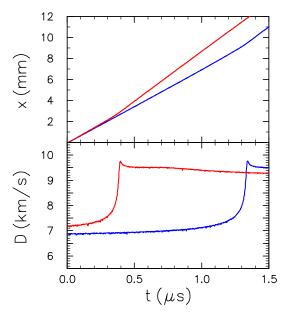
Simulations were performed using the Am<sup>r</sup>i<sup>t</sup>a[3, 4] system with a Godunov based patch integrator on an adaptive Lagrangian mesh. Up to 8 levels of refinement by a factor of 2 were used, starting with a level 0 mesh having a cell size of 0.010 mm. The mesh refinement allows the reaction zone of the detonation wave (about 0.025 mm for PBX 9404) to be well resolved while propagating the shock front for a long distance (up to 14 mm). It also allowed the shock wave in the thin gap (0.030 mm) between the PBX 9404 and the HMX to be well resolved.

Similar constitutive properties were used for HMX — EOS of reactants, EOS products and Arrhenius reaction rate — as those that matched VISAR data from PBX 9501 reaction zone experiments; see [2].

There is a slight difference in the initial density and the specific reaction energy. In addition, the Arrhenius rate constant for HMX is lowered by 40 % compared to that of PBX 9501. For an HMX shock to the PBX 9404 CJ pressure (35 GPa), the change in reaction rate is equivalent to lowering the shock temperature (1448 K) by 50 K. Possibly, the change in temperature is due to a difference in specific heat between the PBX 9404 and the pure HMX.

#### HMX INITIATION WITH FLYER PLATE

Craig's experiments [1, p. 1064] used an explosively driven flyer plate to drive a shock in a magnesium plate abutting a wedge shaped HMX crystal. We note that magnesium is a good impedance match for HMX in the shock pressure range of 30 to 40 GPa. This minimizes reflected waves at the magnesium/HMX interface. Simulations of the lead shock trajectory and its wave speed are shown in fig. 1 for two initiation shock pressures.



**FIGURE 1.** Shock initiation simulations for single crystal HMX driven by shock in abutting magnesium plate. Top figure is trajectory of shock front. Bottom figure is wave speed of lead front. Red and blue curves correspond to initial shock pressure in magnesium of 34 and 30 GPa, respectively.

For the 30 GPa pressure case, initiation requires a run distance of over 9 mm. The experiment used a 7.4 mm crystal and a detonation wave was not observed. By comparison, with a shock pressure of 34 GPa, the HMX transits to a detonation after slightly over 2 mm of run. Again, this is comparable with the experimental observation. Moreover, after transition, the detonation wave is slightly overdriven at a detonation speed of 9.5 km/s. If allowed to propagate long enough, the detonation speed would decrease to the CJ speed of 9.1 km/s. This is slightly larger than the CJ speed of PBX 9404 (8.8 km/s) because of the higher specific reaction energy of the pure HMX.

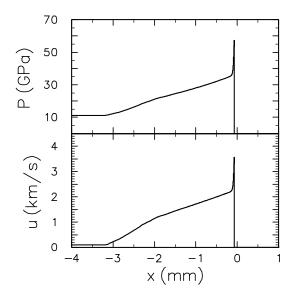
A third experiment at 42 GPa resulted in a prompt detonation. The large variation of run distance to detonation with small changes in shock pressure is a consequence of the sensitivity of the induction time to temperature for an Arrhenius reaction rate.

## **HMX INITIATION WITH PBX 9404**

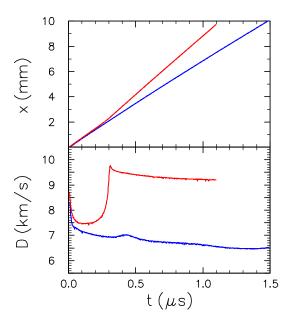
Campbell & Craig's experiments [1, p. 1064] used the breakout of light on the side surface of HMX, recorded with a streak camera, as a measurement of the lead shock trajectory. To prevent radiation from an air shock blinding the camera, the explosive was placed in a tank of water. Consequently, the PBX 9501 surface roughness at the interface with the HMX is modeled as a thin layer of water.

The simulations start just before the PBX 9404 detonation wave reached the HMX. The initial conditions are shown in fig. 2. The reaction zone profile is computed from the ODEs for a steady CJ detonation wave based on the PBX 9404 equation of state and an Arrhenius reaction rate. The following Taylor wave is computed from the characteristic speeds along the isentrope through the CJ state, based on the products equation of state, and assuming that the PBX 9404 was promptly initated and the detonation wave propagated 6 mm.

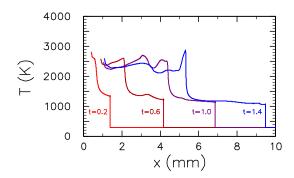
Simulations of the lead shock trajectory in the HMX and its wave speed are shown in fig. 3 for two cases. For the ideal case, without a gap, the HMX is initated within  $0.3 \,\mu s$ . The time to ignition is slightly less than the previous case of a shock at the CJ pressure. This is due to the short duration high pressure pulse from the PBX 9404 reaction zone.



**FIGURE 2.** Initial conditions for initiation simulations driven by PBX 9404 detonation wave. Profile at t=0 consists of resolved reaction zone followed by Taylor wave assuming run distance in the PBX 9404 of 6 mm.



**FIGURE 3.** Shock initiation of single crystal HMX driven by detonation wave in PBX 9404. Top figure is trajectory of shock front. Bottom figure is wave speed of lead front. Red and blue curves correspond to no gap and 30  $\mu$ m water gap, respectively.



**FIGURE 4.** Shock initiation of single crystal HMX driven by detonation wave in PBX 9404. Temperature profiles in the HMX at a sequence of times for case with  $30 \, \mu m$  water gap between the PBX 9404 and the HMX.

In contrast, with a 30 micron water gap, the lead wave speed decreases and is well below the CJ detonation speed after the wave has propagated for 10 mm. The very rapid initial drop in wave speed is due to the narrow reaction zone in PBX 9404. A detailed examination of the numerical results shows that a thin layer in the HMX next to the gap is shocked to a high enough temperature to react after an induction time of about  $0.1 \,\mu s$ . This sends a pressure wave out. However, by the time it catches up with the lead front (indicated by the bump in the wave speed at  $t=0.4 \,\mu s$ ) the shock has weakened sufficiently that the overtaking wave is too little too late to cause a transition to detonation.

Temperature profiles for a sequence of times are shown in fig. 4. The profiles display a two wave structure; lead shock wave followed by a burn front. The burn front is not a deflagration wave as the simulation did not include heat conduction. Rather the burn front is due to the induction time after the shock passage. Complete reaction occurs behind the burn front. Thus, even though the HMX does not detonate, it would burn completely. A possible exception is a neighborhood of the side boundaries where weak confinement would lead to a strong rarefaction that quenches the reaction.

## CONCLUDING REMARKS

Initiation simulations of the gap test are sensitive to the gap thickness and the gradient from the Taylor wave. Moreover, for a homogeneous explosive with a temperature dependent chemical rate, initiation is also sensitive to the equation of state (in particular, the specific heat) and Arrhenius rate parameters. Though the values of the parameters used may be slightly off, the simulations are compatible with initiation experiments using both a uniform drive pressure generated by a flyer plate and a drive with a pressure gradient from a detonation wave. The micro-gap hypothesis is a likely explanation for the failure of a PBX 9404 detonation wave to initiate an HMX crystal.

As a sanity check, Campbell & Craig did an additional experiment in which two samples, one of a single crystal HMX and the other of PBX 9404, were placed on a detonating PBX 9404 booster. The PBX 9404 sample did initiate while the crystal did not. One can infer that with hot spots, nucleated by shock compression of pores, the PBX promptly reinitiates after the gap. But without hot spots, the homogeneous HMX has a long enough induction time such that the Taylor wave lowers the pressure fast enough to prevent the crystal from detonating.

## **ACKNOWLEDGMENTS**

This work was carried out under the auspices of the U. S. Dept. of Energy at LANL under contract DE-AC52-06NA25396.

#### REFERENCES

- 1. Campbell, A. W., and Travis, J. R., "The Shock Desensitization of PBX-9404 and Composition B-3," in *Eighth Symposium (International) on Detonation*, 1986, pp. 1057–1068.
- Menikoff, R., Combustion Theory and Modelling, 10, 1003–1021 (2006).
- 3. Quirk, J. J., "Amrita A Computational Facility for CFD Modelling," in 29<sup>th</sup> Computational Fluid Dynamics, von Karmen Institute, 1998, VKI Lecture Series, chap. 4, URL http://www.amrita-ebook.org/pdf/vki/cfd29/jjq/vki:cfd29::jjq\_11.pdf.
- Quirk, J. J., "AMR\_sol: Design Principles and Practice," in 29<sup>th</sup> Computational Fluid Dynamics, von Karmen Institute, 1998, VKI Lecture Series, chap. 5, URL http://www.amrita-ebook.org/pdf/vki/cfd29/jjq/vki:cfd29::jjq\_12.pdf.